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Spin-polarized ballistic transport channel in a thin superlattice composed of zincblende half-metallic compounds

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We examine theoretically conduction processes near the Fermi energy of thin layers of zincblende structure half metals, using as an example a superlattice consisting of monolayers of GaAs and MnAs, a bilayer of CrAs, and a bilayer of GaAs. By artificially separating bilayers, we show that non-fourfold coordinated Cr states thwart half metallicity. However, capping the metal-As bilayers restores half metallicity and ballistic conduction of electrons around 0.3 eV above the Fermi level will give nearly 100% spin-polarized transmission in the direction of the thin superlattice. Recent developments suggest atomic layer epitaxy can be used to produce such thin layers for spintronics applications.

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One of the most fundamental characteristics of a material is whether it is metallic, or semiconducting or insulating. In 1985, a new class of material was categorized as a half-metal (HM)[1] where electrons with spins polarized in one direction exhibiting metallic properties and spins polarized in the opposite direction showing semiconducting properties. Because of a new development of utilizing electron spins in future electronic devices, referred to as spintronics, this kind of materials has recently instigated vigorous effort by many groups around the world.[2–7]

After the pioneering work of Akinaga *et al.*[2] who predicted the half-metallic behavior for CrAs with zincblende (ZB) structure and then grew it in a thin film form, several other transition metal compounds have been investigated experimentally[3] and theoretically.[4–7] In all ZB transition metal pnictides, the majority spin channel shows metallic properties and the minority spin polarization exhibit semiconducting behaviors when they are half metals[7]. To search for possible new HM materials derived from these ZB-HMs for spintronics applications, studies of heterostructures,[4] and superlattices[8] have theoretically been carried out. Sanvito and Hill[4] have examined the electronic and transport properties of a digital ferromagnetic heterostructure[9] composed of a monolayer of MnAs and 16-layers of GaAs. They found that the conduction is confined in the planar region of MnAs. Experimentally, it has been found that the bilayer CrAs and bilayer GaAs can be best grown in ZB structure to form CrAs/GaAs superlattice by molecular beam epitaxy[10]. On the other hand, the Mn concentration[11] in the diluted magnetic semiconductor GaMnAs can reach up to 10%. Furthermore, ZB MnAs monolayers[9] have been successfully embedded into thick GaAs. Therefore, it would be interesting to theoretically investigate how a thin film superlattice involving HMs to exhibit half metallic properties and show a ballistic transport in the growth direction.

In this paper we address these issues using a thin superlattice made of MnAs, CrAs and GaAs by carrying out first-principles calculations. We start with a model consisting of three separate regions: a region consisting of a monolayer of GaAs and MnAs each, which we denote by $Ga_{0.5}Mn_{0.5}As$, a bilayer region composed of CrAs and another bilayer region of GaAs. To observe the parentage of the important states, we first separate them somewhat, then bring them together to form a model superlattice and address the question of ballistic conduction by examining the charge density from states having energies above the Fermi energy by 0.3 eV. We find that the superlattice is a HM and the ballistic transport is spin selective.

First-principles total energy and electronic structure calculations have been performed using the pseudopotential plane-wave method[12] based on the density functional theory (DFT)[13] within the generalized gradient approximation (GGA).[14] We used the VASP program[15,16] for our calculations in which ultrasoft pseudopotentials[17] are used for Ga, As, Mn and Cr atoms with normal valence electron configurations. Spin polarized calculations were carried out to examine the behavior of different spin channels. The cutoff energy is taken to be 450 eV. The Monkhorst-Pack[18] **k**-point mesh (11x11x7) was used to determine 144 special **k**-points for both the separated and the contact cases. More than 144 special **k**-points were tested that total energy is converged to be better than 1 meV.

To investigate the formation of a conducting channel, we start with a model in which $Ga_{0.5}Mn_{0.5}As$, CrAs, and GaAs are separated into three slab regions. Then, we moved the regions close together until the metal atoms and the Ga atoms in a region forming the respective bulk-like bonds with the As atoms in the neighboring region. The GGA optimized lattice constant of GaAs ($a_o = 5.722\AA$) is used in our superlattice calculations, which is 1% larger than the measured lattice constant. The sectional views of the superlattice are presented in Fig. 1. The unit cell is tetragonal with the lattice constants $a_o/\sqrt{2}$ in the **a** and **b** directions. Fig. 1(a) shows the slab configuration with c to be $4.0 \times a_o$ and Fig. 1(b) the superlattice with c equal to

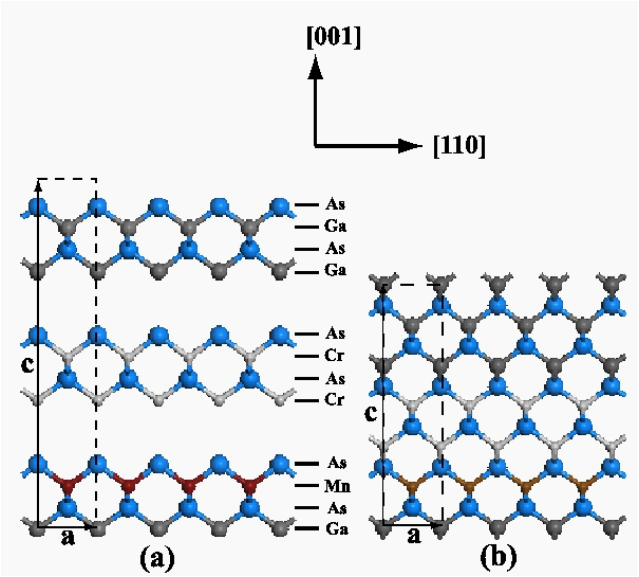

FIG. 1: (a)Separated superlattice; (b)contact superlattice viewed along **b**. **b** is the $[\bar{1}10]$ direction.

$3.0 \times a_o$. By reducing the spacing between the regions from the $4.0a_o$ case to the $3.0a_o$ case, we are able to examine the change of the charge densities between the two cases and whether a conduction channel is formed.

In the $4.0a_o$ case, the system is a ferromagnetic two dimensional metal with the net magnetic moment equal to the $9.11\mu_B$ per unit-cell. The total density of states (DOS) and the projected DOS on the metal atomic sites are shown in Fig. 2. At the Fermi energy E_F, there are densities of states for both majority and minority spin channels. Considering first the total DOS, we find the low-lying, isolated As-*s* states at around -10 eV, the Ga-*s* and As-*p* bonding states at about -6 eV, followed by metal-*d*–As-*p* hybridized states in the vicinity of E_F. The Mn *d*-states are located lower in the energy than the corresponding Cr *d*-states, consistent with nuclear charges. Due to the lack of the four-fold coordination around the interface atoms, the hybridized bonding t_{2g} states, in particular on the Cr atoms, are broadened to contribute the metallic behavior in the minority spin channel. Moreover, the minority spin e_g states located on the Cr atoms contribute a large part of DOS at E_F and thwart half metallicity. The total charge density for the majority and minority spin states in a (114) plane containing the Ga-As-Mn-As, Cr-As-Cr-As, and Ga-As-Ga-As chain are shown in Fig. 3(a) and Fig. 3(b), respectively. There is essentially no overlapping of charges between the regions. We also plot the charge density for the states with energies 0.3 eV above E_F in the (114) plane, shown in Fig. 3(c), which are the states that accommodate externally injected electrons. However, the charge distributions are confined in the three regions because of the energy barriers (vacuum) between the regions. They do not form any channel along the **c**-direction. The only way for an electron to move from one end of the superlattice to another end is

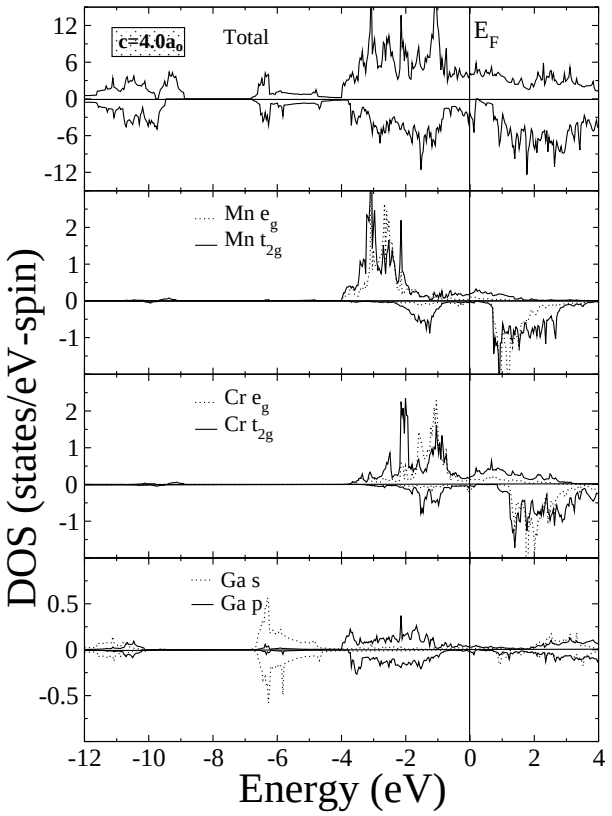

FIG. 2: Total and projected density of states of $(Ga_{0.5}Mn_{0.5}As)(CrAs)(GaAs)$ in the $c = 4.0a_o$ case. The material is metallic. The positive (negative) values represent majority (minority) spin. The Fermi energy is set to zero.

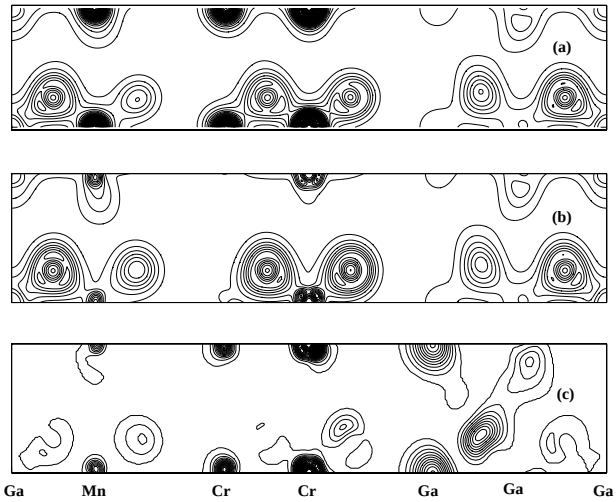

FIG. 3: In the $c = 4.0a_o$ case, the calculated charge density is plotted with contour in the (114) plane for (a) majority spin channel; (b) minority spin channel; (c) states with energies 0.3 eV from the Fermi energy.

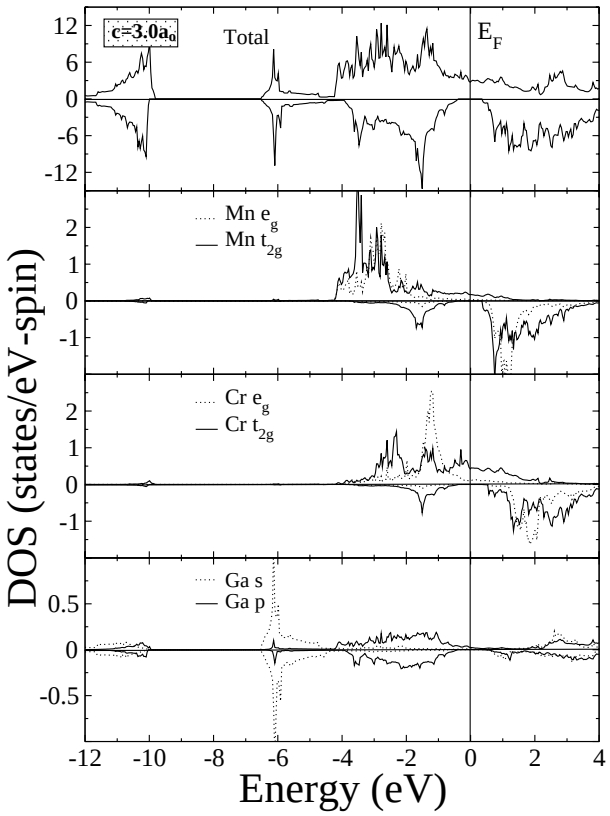

FIG. 4: Total and projected density of states of $(Ga_{0.5}Mn_{0.5}As)(CrAs)(GaAs)$ in the $c = 3.0a_o$ case. The material is half-metallic. The positive (negative) values represent majority (minority) spin. The Fermi energy is set to zero.

by tunneling. Ballistic transport will not be possible.

In the physical realizable $3.0a_o$ case, each atom has four neighbors. Due to the *d*-*p* hybridization between the transition metal elements in one bilayer and the As atoms in the neighboring bilayer and the crystal field effect, the sample is HM with metallic majority spin channel. The magnetic moment is $10\mu_B$ per unit-cell. This value can be accounted for by the formula presented in Ref.[7]. However, it does not mean that the saturation magnetization of the thin superlattice is larger than the transition metal compounds.[8] The semiconducting gap in the minority spin channel is 0.95 eV, which is only slightly less than the ones of ZB MnAs and ZB CrAs. To understand the electronic properties of the $c = 3.0a_o$ case, we show the corresponding total and projected DOS in Fig. 4. The As *s*-states lie near -10.0 eV. The metal-*d*–As-*p* hybridized states are located around 4 eV below E_F. For the majority spin channel, the Mn t_{2g} states at -3.7 eV and e_g states at -2.9 eV are found, while the Cr t_{2g} states are broadened around -2.0 eV with the more localized e_g states at -1.9 eV. For the minority spin channel, the *d* states are shifted relative to the majority by the exchange field of about 3 eV. Because the more localized nonbonding e_g states for Mn and Cr shifted more than the strongly hybridized bonding t_{2g} states, a bonding-nonbonding semiconducting gap is opened at E_F.

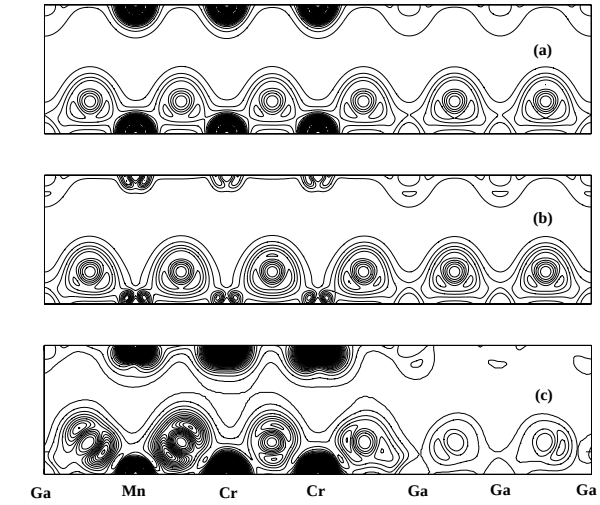

FIG. 5: In the $c = 3.0a_o$ case, the calculated charge density is plotted with contour in the (113) plane for (a) majority spin channel; (b) minority spin channel; (c) states with energies 0.3 eV from the Fermi energy.

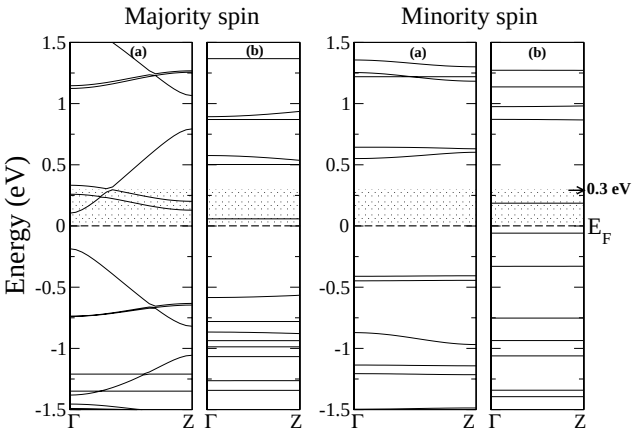

FIG. 6: Band structures along the **c** direction for the thin superlattice: (a) the $c = 3.0a_o$ case; (b) the $c = 4.0a_o$ case. The states with energies 0.3 eV above the Fermi energy are shaded. The horizontal dashed line indicates the Fermi energy.

To examine whether there is a conducting channel in this thin superlattice, we need to focus only on the majority spin states. The minority spin states do not contribute because no state is in the range of 0.3 eV above E_F. First we give the total charge densities in a (113) plane for the majority and the minority spin states in Fig. 5(a) and Fig. 5(b), respectively. The majority charge densities show the Mn,Cr-*d*–As-*p* bonding and the strongly localized e_g density at the Mn,Cr atoms,

consistent with the p-t_{2g} hybridization and the non-bonding character of e_g exhibited in the projected DOS (Fig. 4). The minority charge densities also show the As-p-Mn(Cr)-d bonding with the specific t_{2g} character at the Mn,Cr atoms. The charge densities around the Ga atoms are almost non-spin-polarized. In Fig. 5(c), we give the charge distributions for the majority spin states whose energies are 0.3 eV above E_F. Along the zig-zag chain in the (113) plane, there are contours extending from the left end to the right end. This feature is in distinct contrast to the $c = 4.0a_o$ case. Since these states above E_F are available for any injected electron, one of the states associated with the charge distribution can be occupied when an electron is injected into the left end of the thin superlattice. The probability of finding the electron at the right end is determined by the charge density. The charge density distribution indicates the electronic conducting channel. The electron transport from the left end to the right end should not suffer any scattering. This indicates that a thin superlattice made of $Ga_{0.5}Mn_{0.5}As$, CrAs and GaAs can exhibit spin polarized ballistic transport with a component along the **c** direction. In Fig. 6, we also give the band structures for both cases. Γ-Z is the **c** direction orthogonal to the CrAs plane. In the $c = 3.0a_o$ case, the majority spin bands present a strong dispersion, while in the $c = 4.0a_o$ case, there are flat bands which indicate a weak overlap in this direction and the two-dimensional character. The majority spin conduction states of the $c = 3.0a_o$ case in the shaded area should be responsible for the conducting channel along the **c** direction. A gap of 0.95 eV in the minority spin band shows the thin superlattice of the $c = 3.0a_o$ case is a half metal. It has the feature that the current in the direction of superlattice should be fully spin polarized. As in reference[7,9,10], both transition metal compounds should be able to grow on the substrate GaAs in thin film forms.

In summary, we examine the formation of a channel for 100% spin polarized ballistic transport in a thin superlattice formed by $Ga_{0.5}Mn_{0.5}As$, CrAs and GaAs. By first separating the regions and bringing them together, we illustrate how the completeness of the three dimensional d-p hybridization and the crystal field effect is crucial for the HM properties of the superlattice. A possible channel for ballistic transport of injected electrons is exhibited by calculating the charge distribution from states with the energy 0.3 eV above E_F. The channel has the feature of full spin polarization. We propose that this thin superlattice grown on the substrate GaAs will be an excellent candidate for spintronics application.

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